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Strain Functionals for Characterizing Atomistic Geometries EDWARD KOBER, SVEN RUDIN, Los Alamos National Laboratory — The development of a set of strain tensor functionals that are capable of characterizing arbitrarily ordered atomistic structures is described. This approach defines a Gaussian-weighted neighborhood around each atom and characterizes that local geometry in terms of n-th order strain tensors, which are equivalent to the moments of the neighborhood. Fourth order expansions can distinguish the cubic structures (and deformations thereof), but sixth order expansions are required to fully characterize hexagonal structures. Other methods used to characterize atomic structures, such as the Steinhardt parameters or the centrosymmetry metric, can be derived from this more general approach. These functions are continuous and smooth and much less sensitive to thermal fluctuations than other descriptors based on discrete neighborhoods. They allow material phases, deformations, and a large number of defect structures to be readily identified and classified. Applications to the analysis of shock-loaded samples of Cu, Ta and Ti will be presented. This strain functional basis can also then be used for developing interatomic potential functions, and an initial application to Cu will be presented.

Edward Kober
Los Alamos National Laboratory

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